SECTION II

METHODOLOGY

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2. METHODOLOGY

Air flow and heat transfer within a fluid are governed by the principles of conservation of mass, momentum, and thermal energy. In order to predict the airflow and temperature, as well as the distribution of contaminants at any given point in space, CFD techniques are used to represent the fundamental laws of physics describing fluid flow and heat transfer.

2.1 Methodology Overview

This section outlines the fundamental aspects of CFD, the equations utilized, and the methodology adopted with respect to the problem at hand.

2.1.1 What is CFD?

Computational Fluid Dynamics can be summarized by the following definitions:

Computational

The computational part of CFD means using computers to solve problems in fluid dynamics. This can be compared to the other main areas of fluid dynamics, such as theoretical and experimental.

Fluid

When most people hear the term fluid they think of a liquid such as water. In technical fields, fluid actually means anything that is not a solid, so that both air and water are fluids. More precisely, any substance that cannot remain at rest under a sliding or shearing stress is regarded as a fluid.

Dynamics

Dynamics is the study of objects in motion and the forces involved. The field of fluid mechanics is similar to fluid dynamics, but usually is considered to be the motion through a fluid of constant density.

This shows that CFD is the science of computing the motion of air, water, or any other gas or liquid.

2.1.2 Overview of CFD

The science of computational fluid dynamics is made up of many different disciplines from the fields of aeronautics, mathematics, and computer science. A scientist or engineer working in the CFD field is likely to be concerned with topics such as stability analysis, graphic design, and aerodynamic optimization. CFD may be structured into two parts, generating or creating a solution, and analyzing or visualizing the solution. Often the two parts overlap, and a solution is analyzed while it is in the process of being generated in order to ensure no mistakes have been made. This is often referred to as validating a CFD simulation.

2.1.3 CFD Solutions

When scientists or engineers try to solve problems using computational fluid dynamics, they usually have a specific outcome in mind. For instance, an engineer might want to find out the amount of lift a particular airfoil generates. In order to determine this lift, the engineer must create a CFD solution, or a simulation, for the space surrounding the airfoil. At every point in space around the airfoil, called the grid points, enough information must be known about the state of a fluid particle to determine exactly what direction it would travel and with what velocity. This information is called flow variables.

2.1.4 Governing Equations of Fluid Dynamics

The governing equations of fluid dynamics represent the conservation of mass, momentum, and energy for a fluid continuum. The conservation of mass states that mass cannot be created or destroyed, and the conservation of energy is similar. The conservation of momentum is simply Newton's Law of Motion (force = mass x acceleration) that is cast in a form suitable for fluid dynamics. Because the governing equations are the three conservation laws, they are also referred to as the conservation law equations. The governing equations receive their name because they determine the motion of a fluid particle under certain boundary conditions.

The governing equations remain the same, but the boundary conditions will change for each problem. For example, the shape of the object may be different, or the speed of the undisturbed air may change, and these changes would be implemented through a different set of boundary conditions. In general, a boundary condition defines the physical problem at specific positions. Fundamental boundary conditions include the no-slip condition at the interface between solid and fluid that leads to the formation of a wall boundary layer. Another is the fixed mass outlet where it is ensured that a constant mass flow is extracted from the solution domain at a specified plane.

The governing equations have actually been known for over 150 years. In the 19th century, two scientists, Navier and Stokes, described the equations for a viscous, compressible fluid, which are now known as the Navier-Stokes equations. These equations form a set of differential equations. The generic form of these relationships follow the advection diffusion equation, 2.1:

$$\frac{\partial}{\partial t}(\rho\varphi) + div\left(\rho\nabla\varphi - \Gamma_{\varphi} grad\varphi\right) = S_{\varphi} \qquad (2.1)$$

transient + advection - diffusion = source

The variable phi (φ) represents any of the predicted quantities such as air velocity, temperature, or concentration at any point in the 3-dimensional model. All subsequent terms are identified in section 2.6. This equation is derived by considering a small, or finite, volume of fluid. The left hand side of the equation refers to the change in time of a variable within this volume added to that advected into it, minus the amount diffused out. This is in turn equal to the amount of the variable flux (i.e. momentum, mass, thermal energy) that is added or subtracted within the finite volume. Though deceptively simple, only the emergence of ever faster computers over the past two decades has made it possible to solve the real world problems governed by this equation.

Despite their relatively old age, the Navier-Stokes Equations have never been solved analytically. The numerical techniques used to solve these coupled mathematical equations are commonly known as computational fluid dynamics, hence CFD for short. At the present time, CFD is the only means for generating complete solutions.

The Navier-Stokes Equations are a set of partial differential equations that represent the equations of motion governing a fluid continuum. The set contains five equations, mass conservation, three components of momentum conservation, and energy conservation. In addition, certain properties of the fluid being modeled, such as the equation of state, must be specified. The equations themselves can be classified as non-linear, and coupled. Non-linear, for practical purposes, means that solutions to the equations cannot be added together to get solutions to a different problem (i.e., solutions cannot be superimposed). Coupled means that each equation in the set of five depends upon the others, so that they must all be solved simultaneously. If the fluid can be treated as incompressible and non-buoyant, then the conservation of energy equation can be de-coupled from the others and a set of only four equations must be solved simultaneously, with the energy equation being solved separately, if required.

The majority of fluid dynamics flows are modeled by the Navier-Stokes equations. The Navier-Stokes equations also describe the behavior of turbulent flows. The many

scales of motion that turbulence contains, especially its micro-scales, cause the modeling of turbulent processes to require an extremely large number of grid points. These simulations are performed today, and fall into the realm of what is termed Direct Numerical Simulations (DNS). These DNS simulations are currently only able to model a very small region, in the range of 1 sq. ft., using current supercomputers. Differential equations represent differences, or changes, or quantities. These changes can be with respect to time, or with respect to spatial locations. For example, in Newton's Law of Motion (F = ma), the time rate of change of velocity, or acceleration, is equal to the force/unit mass. If the quantities depend on both time and space, the equations are written to take this into account, and are known as partial differential equations, or PDE's. In most general formulations, the governing equations for physical phenomena are written in terms of rates of change with respect to time and space, or as partial differential equations.

2.1.5 Flow Variables

The flow variables contain the information about the fluid state at a point in space. Enough information must be maintained in order to specify a valid fluid state; i.e., two thermodynamic variables, such as pressure and temperature and one kinematic variable, such as velocity (note that a velocity will usually have more than one component, i.e., in three dimensions it will have three components).

In this research the variables under consideration are the three components of velocity, pressure, temperature, concentration, and two variables characterizing turbulent levels: turbulent kinetic energy and its rate of dissipation.

Over the past 25 years, CFD techniques have been used extensively and successfully in the mainly high-end sectors, such as the nuclear and the aerospace industries. In its raw and general form, CFD has always been the forte of fluids experts. However, recently the concept of tailoring CFD software, combined with the appropriate expertise in the market segment being addressed, specifically building heating and ventilation, has made it possible to apply these powerful methods to provide fast and accurate results to designers under severe time and budgetary constraints. In fact, this project would not have been practical without these new elements in place.

2.1.6 How Does it Work?

In order to generate a CFD solution, two processes must be accomplished, namely;

- geometry definition and grid generation
- numerical simulation

In broad terms, grid generation is the act of specifying the physical configuration to be simulated and dividing it up into a three dimensional grid containing a sufficient number of small regions known as control volume cells so that the Navier-Stokes partial differential equations can be solved iteratively. Numerical simulation is the process of applying a mathematical model to that configuration and then computing a solution. These two stages are sequential, the grid generation being performed before any numerical simulation work can be done.

2.1.6.1 Grid generation

Grid generation is the process of specifying the position of all of the control volume cells that will define both the physical configuration to be simulated, and the space surrounding it. Grid generation is one of the more challenging and time consuming aspects of CFD because it involves creating a description of the entire configuration that the computer can understand. The model thus defined must include the relationship with the space surrounding the chosen model as well as the surfaces and processes contained within it. In both cases the most important factor is to maintain a suitable number of control volume cells in areas where there will be large or rapid changes occurring. These changes may be changes in geometry, such as a sharp corner of an object, or they may be sharp changes occurring in the flow field about the object, such as the edge of jet issuing from the diffuser. This is called maintaining a suitable grid resolution. Without a suitable grid resolution, valuable information can be lost in the numerical simulation process, and the resulting solution can be misleading. Determining what exactly constitutes enough grid resolution is one of the most important jobs a CFD scientist or engineer must perform. While too few control volume cells can lead to useless simulations, too many control volume cells can lead to computer requirements that can't be fulfilled (example: trying to run the latest version of Microsoft Word on a 286 chip).

2.1.6.2 Numerical simulation

As with every other aspect of CFD, the numerical simulation process can also be broken into two steps,

1) <u>Modeling the Physics</u>

If the user does nothing else, then the boundary surfaces of the solution domain are "zero flow" (i.e., symmetry surfaces). These have zero mass flow, zero surface friction and zero heat transfer. The interior of the domain contains only fluid as defined by the properties (such as density, viscosity, etc.). Anything else (e.g., inflow or outflow, walls, internal objects, heat gains or losses) must be specified explicitly by the user. These are known as boundary conditions.

The locations of boundary conditions are defined in terms of six spatial coordinates (say xS, xE, yS, yE, zS, zE), in meters, referenced from the origin located on one corner of the solution domain. In the case of a two dimensional planar (flat) boundary condition (e.g., the shelves) the orientation is specified and the six coordinates degenerate to five. Additionally, some planar boundary conditions should only affect the fluid (e.g., an external boundary wall has only one surface present in the solution domain).

For accurate geometrical representations, the grid lines (surfaces of the control volume cells) can be forced to align with a boundary condition. If this is not done then the boundary condition will "snap" to the nearest grid line in the final model. This type of allowance is often acceptable when setting up room geometries as the exact location of an item need not be clearly defined.

Below is a list, with a brief description, of the boundary conditions relevant to the approach taken in this study, referred to in the sections of this report.

Rectangular Obstructions	Rectangular obstructions are three dimensional solid rectangular objects, with faces aligned with x, y and z. Friction at all surfaces exposed to fluid is included. There are a number of possible thermal specifications: • Fixed uniform heat flux at all surfaces • Fixed uniform surface temperature • Solve in solid (to investigate conduction through solid)

External Walls	External walls are walls at the edges of the solution domain - or exceptionally internal walls for which solution is required only on one side and "external" conditions can be applied on the other side. Surface friction is evaluated automatically and there are a number of thermal options: • Prescribed heat flux • Prescribed inner wall surface temperature • Prescribed external temperature with detail of the heat transfer through the wall.
Exhausts	Exhausts represent any outflow of air usually when driven using mechanical means. The flow rate is specified as: • Fixed mass flow rate (kg/s) • Linear pressure drop / flow rate fan characteristi • External static pressure
Openings	Openings are any opening through which fluid can enter or leave the domain as a result of pressure differences. The temperature and angle of flow of incoming air can be specified. It is also possible to represent, for example, a grille across the opening by setting a pressure drop (see **Resistances**).

Resistances	Resistances cover any kind of flow resistance (i.e. pressure drops) caused by porous items within the flow domain Two options are available: **Planar resistances:** These provide for areas where the resistance is thin and can be applied in one plane. The pressure drop is given by the expression: $DP = f \frac{1}{2} \rho (v/b)^2$ Where DP Pressure drop f loss coefficient *v* velocity of fluid b geometrical free area ratio of obstruction **Volume resistances:** These provide for areas where the resistance occupies a significant thickness in the solution domain and resistance will occur in more than one direction. The pressure drop is the same as for a planar resistance except that it is expressed as pressure drop per meter and the factor and free area ratio is required for each co-ordinate direction. **Loss Coefficient and Free Area Ratio:** The loss coefficient will depend upon the actual geometry of the item causing the pressure drop. This will be obtained from experiment or empirical relationships in text books. Care is needed as it may be set with respect to an approach velocity or device velocity. If the latter is chosen then there will be an associated free area ratio so that the program can correctly calculate the pressure drop. The free area ratio is not required if the setting is based upon the approach velocity.

Sources	Planar and volume sources provide regions of defined source of heat or momentum, or fixed values of velocities, concentration, and / or temperature. The following options are available: • Prescribed source of heat, concentration, and / or momentum • Fixed values of velocity, concentration, and / or temperature • Linear source of heat, concentration, and / or momentum given by the expression: *source = coefficient (value - velocity or temperature)*
Supplies	Supplies are to bring air in from outside, normally conditioned air from the main plant. The flow is set using: • Fixed mass flow rate (kg/s) • Linear pressure drop / flow rate fan characteristic The temperature and angle of flow of incoming air can be specified.
Thin Walls	Internal thin walls are thin solid surfaces within the solution domain and aligned with the grid. Solution is carried out on both sides. The walls are impervious to flow but it is possible to specify heat transfer across them. Surface friction (different on each side if required) is evaluated.
Triangular Prisms	Triangular prisms are solid objects with triangular cross section, and with all faces except the sloping face aligned with x, y and z. All surfaces are zero friction and only the sloping surface has heat transfer. This is specified in terms of a temperature and heat transfer coefficient, or, as a fixed heat flux.

2) Numerically Solving the Physical Model

Integration is one of the cornerstones of calculus, the other being differentiation. In order to find the solution domain (area under a solution curve) numerically, the curve would be chopped up into little pieces, and then the area under each little curve would be approximated. The sum of all of the approximate little areas will be close to the actual area under the curve. The difference between the actual and approximate areas is the numerical error and the object is to make this error so small it isn't noticeable. In CFD, rather than integrating a relatively simple function like the equation for a curve, the governing equations of motion for a fluid continuum are integrated.

Let us consider a typical laboratory. The objective is to predict airflow, temperature, and concentration of any airborne contaminant at any point in the laboratory space.

Figure 2.01 shows a set of design parameters such as

the *geometry and layout of the laboratory*.....,
the *sources of heat and contaminants*, ...
as well as the position of *exhaust and ventilation systems.*

In order to do this *the 3-dimensional space* of the laboratory is subdivided into a large number of *control volume cells* (figure 2.02). The size of the cells will influence the detail and accuracy of the final results. This figure is schematically representative of the grid used in this study, though considerably coarser. In most cases the number of cells will run into tens or perhaps hundreds of thousands.

The equations in each cell will subsequently represent the mathematical definition of the equipment and phenomena contained within it. For example, a cell could encompass a volume that envelopes :

a *corner of a piece of furniture.....*
or some heat source.....
or just some air.....

The CFD software will then attempt to solve the Navier-Stokes equation for a pre-determined set of variables for each cell. In a typical three-dimensional calculation these variables would represent :

- *velocities in three directions;*
- *temperature;*
- *pressure;*
- *concentration; and the*
- *turbulence quantities.*

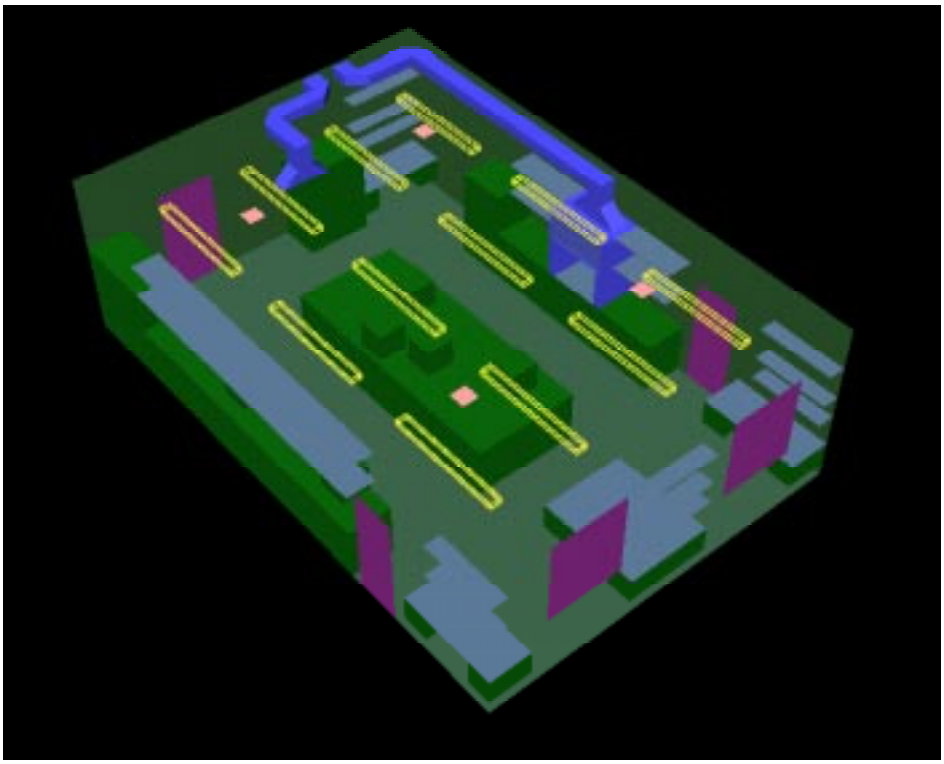

Figure 2.01 *Geometric model.*

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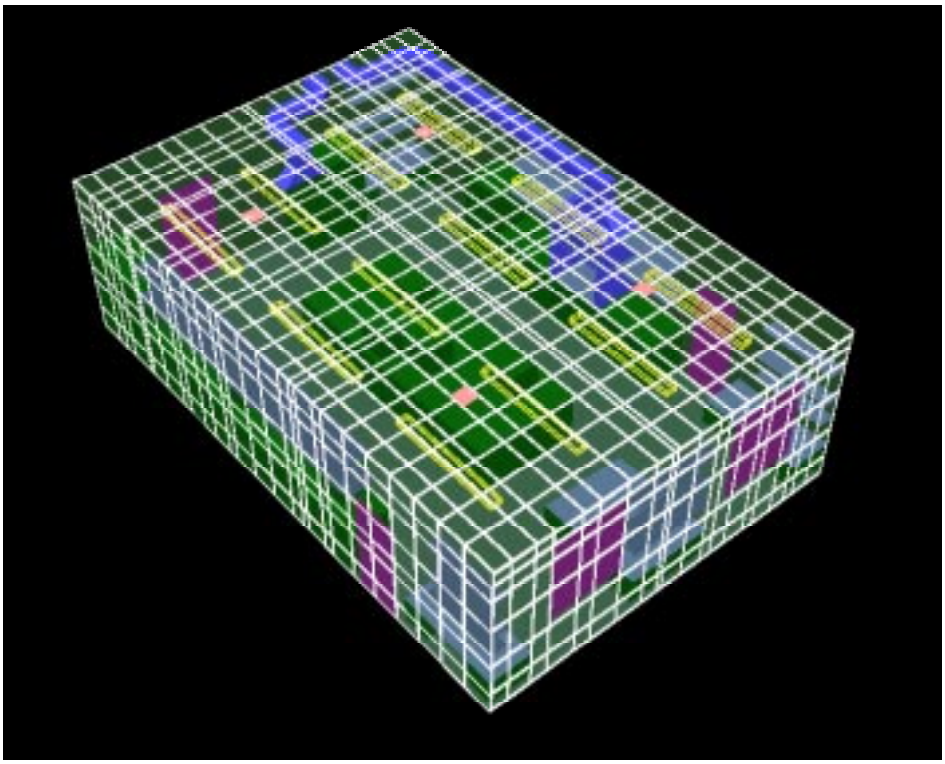

Figure 2.02 *Control volume cells.*

Note that the solution for each variable will depend on the solution for each and every variable in the *neighboring cells and vice versa.* The laws of physics based upon the *conservation of mass, conservation of momentum, and conservation of energy* must be preserved at all times. In this approach, turbulence is modeled using the well established and robust two parameter method known as the k-epsilon model where k represents the kinetic energy and epsilon represents the rate of dissipation.

The mathematical solution is highly iterative, with each iteration resulting in a set of errors. At the end of each iteration the errors for each variable are summed and plotted against iteration number (figure 2.03). A solution is reached when the sums of the errors for each and all the variables reaches a pre-determined and acceptable level.

Each cell within the solution domain has 8 equations associated with it (pressure, three velocities, temperature, two turbulence quantities, and concentration). A laboratory model in this research typically has 80,000 to 100,000 cells. This results in 640,000 to 800,000 equations that have to be solved iteratively until the convergence criteria is satisfied. This is an extremely computer intensive operation that requires the use of powerful state-of-the-art workstations.

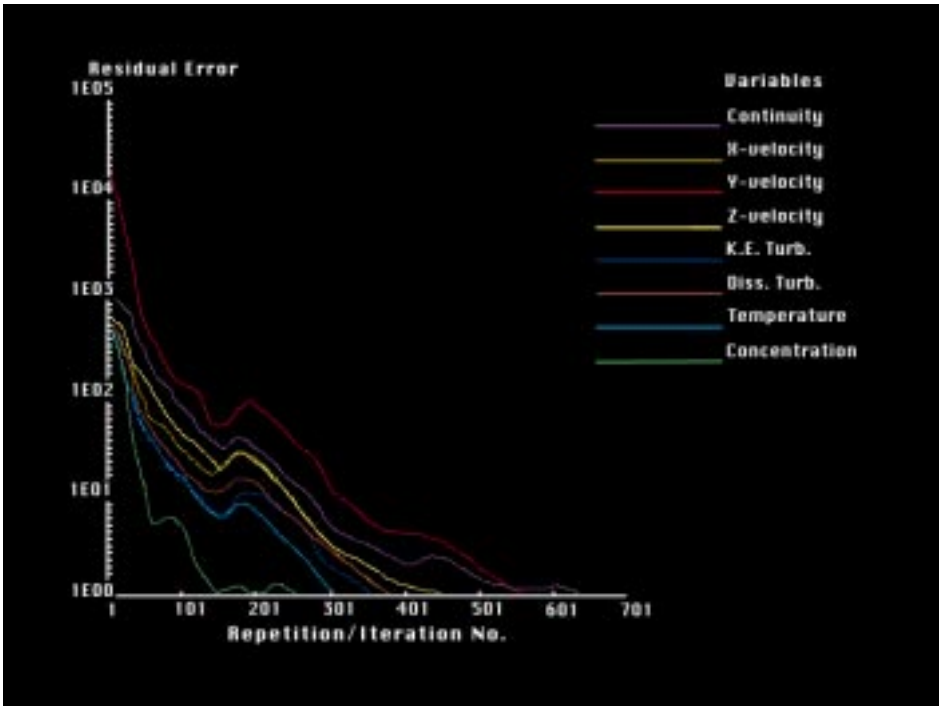

Figure 2.03 *Iterative convergence history of a simulation.*

2.2 Description of Mathematical Model

2.2.1 Governing Equations

The generic form of the governing equations, shown by equation 2.1, can be expanded to form the three fundamental conservation laws that comprise the Navier-Stokes equations. These are the conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0 \qquad (2.2)$$

the conservation of momentum:

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho U_i U_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial U_i}{\partial x_j}\right) + g_i\left(\rho - \rho_0\right) \qquad (2.3)$$

and the conservation of thermal energy:

$$\frac{\partial \rho H}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho U_i H\right) = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \frac{\partial P}{\partial t} \qquad (2.4)$$

These equations describe the behavior of fluids under both laminar and turbulent flow conditions. One of the most important physical effects when calculating the flow in the built environment is that of turbulence. This is particularly so in the laboratory because the leakage at the hood face can normally be entirely accounted for by turbulent diffusion back against the fast inward moving convective flow.

2.2.2 Turbulence Modeling

For this project, a well established and reliable approach to turbulence modeling is required to achieve the large number of calculations necessary for analysis of the many configurations. This section provides some background on the different approaches to modeling turbulence.

To model a turbulent flow, the temporal terms of equations 2.2, 2.3, and 2.4 would have to have a time step (*dt*) small enough to capture all turbulent fluctuations on even the smallest time scales. The same applies to all physical dimensions of the control

volume cells (dx_i) terms. They would have to be as small as that known as the Kolmogarov scale, which decreases non-linearly with an increase in Reynolds number.

To overcome these limitations, variables are split into a mean and fluctuating component, i.e.:

$$U = \overline{U} + u'$$
$$H = \overline{H} + h' \qquad (2.5)$$

These are then substituted back into the instantaneous momentum equation producing the following:

$$\frac{\partial}{\partial x_j}\left(\rho \overline{U}_i \overline{U}_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \overline{U}_i}{\partial x_j} - \rho \overline{u_i' u_j'}\right) + g_i\left(\rho - \rho_0\right) \qquad (2.6)$$

This is known as the time averaged momentum equation. A similar equation exists for the enthalpy equation:

$$\frac{\partial}{\partial x_i}\left(\rho \overline{U}_i \overline{H}\right) = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial \overline{T}}{\partial x_i} - \rho \overline{u_i' h'}\right) \qquad (2.7)$$

The extra terms are produced by this substitution are:

- Reynolds stress = $\rho \overline{u_i' u_j'}$
- Reynolds flux = $\rho \overline{u_i' h'}$

A turbulent flow is characterized by the dominance of diffusion due to the Reynolds stresses and fluxes over the diffusion due to the laminar viscosity or laminar diffusivity of the fluid. The ability of a laboratory hood to contain a contaminant is defined by the ratio of the convective inflow into the hood versus the turbulent diffusion of a contaminant spreading back against the predominant inflow direction. The role of turbulence modeling, to calculate the Reynolds stresses and fluxes, is therefore of vital importance in the accurate prediction of the efficiency of the laboratory hood.

The introduction of the Reynolds stresses and fluxes after decomposition of the turbulent fluctuating variables means that the equation set is now not closed. Some form of closure is required to model these fluxes and stresses. There have been a wide range of methods used to do this, varying from the most simple zero-equation models to the much more complex Reynolds stress transport equations. Figure 2.04 shows how these turbulence models relate to each other.

At the center of the zero-, one-, and two-equation models lies the analogy that where a laminar stress exists, then so can an equivalent turbulent stress (i.e. , Reynolds stress). A laminar shear stress is defined as:

$$\tau = \mu \frac{\partial U_i}{\partial x_j} \qquad (2.8)$$

So, if a fluid can have a laminar viscosity, μ, then a turbulent flow should have a turbulent or eddy viscosity, μ_T. By using the eddy viscosity hypothesis, which Boussinesq proposed, we can relate the Reynolds stress to the mean strain by:

$$-\rho\overline{u_i' u_j'} = \mu_T \left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i} \right) - \tfrac{2}{3}\rho k \partial_{ij} \qquad (2.9)$$

A zero equation turbulence model simply sets a constant value of the eddy viscosity, or deduces it as an algebraic function of flow parameters. A one equation model uses a differential equation to predict one part of the eddy viscosity while a two equation model uses two differential equations.

The main limitation imposed at this stage by equation 2.9 is that the eddy viscosity is the same in all directions at any point. Now, where this may be true of laminar viscosity, which is a property of the fluid, it may not be true of turbulent viscosity, which is effectively a property of the flow. Therefore, this eddy viscosity can have differing values in relation to differing Reynolds stresses. This occurs when the turbulence is said to be anisotropic. Conditions that under certain circumstances may cause anisotropy, and thus could invalidate the isotropic assumption of equation 2.9, include extreme streamline curvature, swirl, adverse pressure gradients, and buoyancy.

The two-equation approach including the standard *k*-ε model and the RNG *k*-ε model variant is presented first. Reynolds stress modeling is then discussed and finally the modeling of the Reynolds fluxes is briefly outlined.

2.2.2.1 k-ε turbulence model

The eddy viscosity is defined from dimensional analysis as:

$$\mu_T = C_\mu \rho \frac{k^2}{\varepsilon} \qquad (2.10)$$

The transport equations for *k* and ε are:

$$\frac{\partial \rho U_i k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right) + P + G - \rho\varepsilon \qquad (2.11)$$

$$\frac{\partial \rho U_i \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right) + C_1\frac{\varepsilon}{k}\left(P + C_3 G\right) - C_2\rho\frac{\varepsilon^2}{k} \qquad (2.12)$$

where P is the shear production defined as:

$$P = \mu_{eff}\frac{\partial U_i}{\partial x_j}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \qquad (2.13)$$

G is the production of turbulence kinetic energy due to buoyancy, and is given by:

$$G = \frac{\mu_{eff}}{\sigma_T}\beta g_i\frac{\partial T}{\partial x_i} \qquad (2.14)$$

C_μ	0.09
C_1	1.44
C_2	1.92
C_3	1.0
σ_k	1.0
σ_ε	1.217

This model has been tried and tested for a whole range of engineering applications. It is simple, but more importantly, it is *stable*. Only two extra differential equations are introduced and the convergence process is less prone to divergence than other, higher order turbulence models. This is the approach adopted for the present research.

2.2.2.2 Re-normalized group theory (RNG) kε turbulence model

Essentially, this model has much the same form as the standard model. It is part empirical and part analytical. The only changes are a modified term relating to the

production of energy dissipation in the ε equation and a different set of model constants. This RNG model is typical of those offered by some commercial general purpose CFD codes. The new equations for *k* and ε become:

$$\frac{\partial \rho U_i k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right) + P + G - \rho\varepsilon \qquad (2.15)$$

$$\frac{\partial \rho U_i \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right) + (C_1 - C_{1RNG})\frac{\varepsilon}{k}(P + C_3 G) - C_2\rho\frac{\varepsilon^2}{k} \qquad (2.16)$$

The new function C_{1RNG} is given by the equations:

$$C_{1RNG} = \frac{\eta\left(1 - \eta/\eta_0\right)}{\left(1 + \beta\eta^3\right)} \qquad (2.17)$$

and:

$$\eta = \frac{k}{\varepsilon}\sqrt{\frac{P}{\mu}} \qquad (2.18)$$

In this case η_0 and β are additional model constants, and the latter should not be confused with the coefficient of thermal expansion. The main modification is to the ε equation where the rate of strain of the flow has been incorporated into the model constants. Under conditions of extreme strain the eddy viscosity is reduced. It is this feature of the RNG model that is said to accommodate *strong* anisotropy in regions of large shear, i.e. the treatment of massive separation and anisotropic large-scale eddies. Most validation of this model has been only under these extremely high strain conditions such as internal flow in a 180° bend and flow within a contracting-expanding duct. Accurate prediction of separation regions seems to be the grail of the validation work. A more realistic range of *softer* type flows (i.e. less extreme strain) has not been studied with the RNG model. It is because of the infancy of this approach that it has not been incorporated at this stage. As and when the model becomes as tried and trusted as the present standard *k*-ε model it will be given greater attention.

2.2.2.3 Reynolds stress models (second order closure models)

Instead of employing the eddy viscosity assumption, which assumes an equal eddy viscosity in all three spatial directions, a Reynolds stress model has an equation for

each of the six Reynolds stresses themselves. This allows the modeling of the transport of each of these individual stresses. This is the most complex of all models and suffers accordingly. Instead of two extra equations we now have an extra seven (an equation for ε is still required as it pops up in the stress transport equations). Convergence stability now becomes a serious problem. Even if convergence is achieved, it normally takes considerably longer than with a two-equation model. Prescription of boundary conditions is also tricky. Instead of setting just *k* and ε, we now have to set values at supply boundaries of all stresses, not the easiest of parameters to obtain from experimental measurement. The question has to be asked as to whether the added theoretical capabilities of an RSM are worth the increased solution time and decrease in stability.

2.2.2.4 Modeling of Reynolds fluxes:

The velocity-enthalpy correlations known as the Reynolds fluxes use much the same methodology as the Reynolds stresses. An eddy diffusivity is therefore defined as:

$$-\rho\overline{u_i' h'} = \Gamma_T \left(\frac{\partial \overline{T}}{\partial x_i} \right) \qquad (2.19)$$

where this eddy diffusivity is related to the eddy viscosity by:

$$\Gamma_T = \frac{\mu_T}{\sigma_T} \qquad (2.20)$$

where σ_T is the turbulent Prandtl number having a fixed value of 0.9. The next step up, as with a second order closure model, is to calculate each of the three fluxes from their own transport equations.

2.2.3. Near Wall Treatment

Fluid velocity at a wall surface is zero, which is known as the no-slip condition. The type of flow between the wall and the bulk flow is known as a shear layer, in this case a wall boundary layer. The boundary layer is a very complex region of high velocity gradient and diffusion dominated development. To model it precisely would necessitate an extremely fine grid. An empirical relationship is therefore used to describe the shape of the boundary layer so that only one grid cell near the wall is required. This empirical relationship describes the shape of the boundary layer in non-dimensional terms. Two non-dimensional terms are formulated. These are the friction velocity:

$$u_\tau = \left(\frac{\tau_w}{\rho} \right)^{1/2} \tag{2.21}$$

and a nondimensionalized distance from the wall (which can be viewed as a local Reynolds number):

$$y^+ = \frac{u_\tau y \rho}{\mu} \tag{2.22}$$

These formulae are based upon the well-established 'universal' relationships:

$$\text{For } y^+ > 11.5 \text{ (turbulent):} \quad \frac{u}{u_\tau} = \frac{1}{0.435} \ln\left(9 y^+\right) \tag{2.23}$$

$$\text{For } y^+ < 11.5 \text{ (laminar):} \quad \frac{u}{u_\tau} = y^+ \tag{2.24}$$

All that is required to calculate the near wall velocity is therefore the distance from the near wall cell center to the wall itself.

2.2.4 Treatment of a Passive Contaminant

A contaminant that is both advected and diffused by the fluid in which it is suspended can be modeled via the introduction of an additional transport equation. This contaminant is passive as it does not effect the fluid flow itself. It is introduced to visualize the effects of a contaminant that is deposited in the plane of the laboratory hood opening. A passive contaminant follows the standard advection - diffusion equation. A concentration, *C*, obeys the time averaged equation of the conservation of concentration flux such that:

$$\frac{\partial}{\partial x_i}\left(\rho \overline{U}_i \overline{C}\right) = \frac{\partial}{\partial x_i}\left(D \frac{\partial \overline{C}}{\partial x_i} - \rho \overline{u_i' c'} \right) \tag{2.25}$$

The velocity / concentration correlation, like the equivalent velocity / enthalpy correlation of equation 2.17, also follows a gradient hypothesis. In this case a turbulent concentration diffusivity is calculated by:

$$D_T = \frac{\mu_T}{Sc_T} \qquad (2.26)$$

Both the laminar and turbulent diffusivities have a value of 1.0.

2.3 Grid Dependency

When performing a CFD investigation it is essential that the computational grid used is of sufficient resolution to ensure accurate results. If a grid is not fine enough in a region of high gradient, the result is a predicted gradient that is smoothed , or diffused, artificially. This effect is called numerical, or false, diffusion.

To overcome this potential source of error, a set of tests is conducted on a typical laboratory model. The grid density alone is increased, keeping all other boundary conditions fixed. The results are then analyzed from each grid density test case and compared. Grid independence is achieved when the results no longer significantly vary with successive increases in grid density. As soon as the results no longer change the effects of numerical diffusion have been minimized. Optimized grid selection is a balance between a non-diffusive grid and one that does not have an excessive number of grid cells.

2.4 Validation

To provide a base line for the CFD simulation, a field measurement program was conducted within a laboratory at the National Institutes of Health. The study was conducted by obtaining velocity data at approximately 200 points within the lab.

The lab is about 10 feet by 15 feet in size, with a ceiling height of 8 feet 8 inches. The door is located at the front left of the room, and the fume hood at the back left. The fume hood is a constant flow system exhausting at a rate of approximately 750 cfm. Supply air to the room is provided by a 24"x24" Titus ceiling diffuser supplying air at a rate of 270 cfm. Additional supply air enters the room via a transfer grill located immediately above the doorway (approximately 150 cfm.) and through various other entrance points such as the cracks around the edges of the doorways and through the cabinets and ceiling.

Prior to the actual field measurement, the lab was outfitted to give the appearance of typical laboratory operating conditions. The shelves were stocked with mockups of lab equipment, and a model desk was constructed of cardboard in the center of the room. Supply and exhaust flows were characterized using two hand-held hot wire flow

measurement devices. Extensive measurements with these devices were conducted along the diffuser outlet, the face of the transfer grill, the face of the fume hood, and the cracks around the doorway. Where possible, the flows were measured directly by means of a flow measurement hood.

After completion of the flow tests, the following air flow balance within the lab was established:

Exhaust:

Fume hood:	750 cfm.

Supply:

Diffuser:	270 cfm.
Transfer grill:	150 cfm.
Leakage at doorway:	100 cfm.
Other leakage:	230 cfm.

The other leakage effects were investigated and identified as entering the room primarily through the tiles in the ceiling.

The principal measurement device for the flow velocities was a Dantec 54N50 Hot Film Low Velocity Flow Analyzer Mark II, which provides velocity measurements accurate to within 5% between a range of 1 cm/s to 30 cm/s.

Over the course of the study, the seating positions of the two operators in the lab remained fixed to eliminate flow variations caused by different positions. During actual sampling periods the operators remained motionless.

The Dantec probe was adjusted to provide velocity sampling for a period of 60 seconds. For each sampling period, the following six measurements were taken:

mean value of velocity;
rms of velocity;
the ratio of the rms to the mean (turbulence intensity);
the 5^{th} percentile of velocity;
the 95^{th} percentile of velocity; and
the temperature.

At each sampling point, measurements were taken at least two times and up to four times. This procedure was adopted in order to ensure that the flow conditions within the lab had reached steady-state conditions after the field operators had stopped

moving within the lab. Any lack of repeatability between samples, or any unduly high turbulent fluctuations, resulted in another sample being taken.

The data were logged onto a spreadsheet on a laptop personal computer. The spreadsheet was configured to allow an on-line inspection of the data points, thus enabling a constant quality assurance check.

A grid of points was established within the room with a spacing of approximately two feet. In regions of high flow, such as the plane of the diffuser, a finer network of points was adopted. In regions of low flow, such as the area near the floor, a coarser grid was used.

The comparison of results between the actual measurement and the CFD results ranged from 3 to 10% in the hood region. The degree of consistency between the measured data and generated CFD result was considered sufficient to proceed with the research.

2.5 Analysis of Simulations

This section details the analysis carried out on the results in order to be able to assess the effect of variations. A CFD analysis produces a vast amount of data. At each grid cell values for pressure, three velocities, turbulence quantities, temperature, and concentration are generated. To obtain a similar quantity of data from a physical model, using probes and thermocouples, would be near impossible. CFD data by itself, in raw form, is not always very useful. The data has to be analyzed in such a way as to produce quantities that characterize the performance of the laboratory hood. This analysis takes place after a simulation has been completed.

A number of techniques were identified as possible methods for identifying hood performance and a FORTRAN post-processor was written to read the simulation results. In fact there are several performance questions that need to be answered in respect of performance. These are as follows :

- What is the likely effect of room airflow on hood containment ?
- What is the performance in terms of laboratory scavenging ?
- Is the environment still satisfactory for occupants ?

While CFD provides a wealth of information that is normally inspected visually, an application such as this with small deviations of complex flow distribution significantly affecting performance, only a numerical analysis of the flow around the hood face can be expected to differentiate between better and worse designs.

The latter two performance questions above can be answered in terms of the level of contamination from the hood based on the leakage getting from the hood into the laboratory. The techniques described here analyze the flow around the hood in order to quantify the effect of the room air movement in terms of its disruption of the flow. To facilitate such an analysis, the progress meeting participants in this project identified a rectangular working zone around the hood face. This working zone represents the region in which the scientist would work and breathe and has a volume defined as the region outside the sash opening to a distance of approximately 1 ft into the laboratory. The surface of this working zone, or box, at the open sash represents the surface through which contaminants must travel in order to escape from the hood. The remaining five surfaces represent the surface through which contaminants must travel in order to move from the working zone into the main laboratory. The latter dictates the level of contamination of the overall environment, and quantifies the ability of the hood to exhaust contamination that has previously escaped from the hood into the working zone.

The following techniques represent methods for identifying disruption of the 'good flow regime' into the hood. All were evaluated for each simulation but not all were used for the final conclusions.

2.5.1 Dalla Valle

The technique identified as Dalla Valle in this project is based on the work identifying the characteristics of a perfect exhaust. The assumption is that a fume hood when undisturbed will have a performance similar to that of a perfect exhaust, and that the difference represents the degree of disturbance caused by the external influences in the laboratory. Dalla Valle derived formulae for square and rectangular openings so that the velocity at any point along the x-axis (perpendicular to the hood face in this instance) may be determined from the following equation:

DALLA VALLE EQUATION

$$\frac{Y}{100-Y} = \left[\frac{0.0833}{1+0.259\left(1-r/r\right)^{1.105}}\right] A^{1.04} x^{-1.91} \qquad (2.27)$$

Subsequent work by F. Memarzadeh (1992) calculated these data for the five surfaces of the box representing the interface of the working zone with the room. The hypothesis is that the extent of the deviation from this distribution characterizes the variation from the perfect hood and an increased loss of containment.

The performance was assessed as follows :

Calculate mean, standard deviation, minimum, and maximum of

$$(V - DV) \tag{2.28}$$

and

$$\frac{(V - DV)}{DV} \tag{2.29}$$

Where

V is the CFD calculated velocity

DV is the 'perfect velocity' predicted by Dalla Valle / F. Memarzadeh.

The advantage of this approach is that it is based on a recognized methodology. It is a comparison with the symmetrically distributed flow through a rectangular exhaust (i.e. the perfect velocity), which can be considered an advantage or a disadvantage since the results will be strongly dependent on the laboratory hood design. The disadvantage is that the latter distribution is opening size dependent and as such requires a different reference for every different hood size or sash opening.

2.5.2 Performance Index

The performance index was developed to account for both the air velocity and the turbulence in the region around the face of the laboratory hood. The intention was to calculate an index that would rise as any:

- reverse flows developed.
- velocity deviated from the mean design face velocity into the sash opening.
- the turbulence intensity increased.

The formulation of the index was as follows

$$\mathrm{PI} = \frac{1}{\mathrm{N}} \sum_{1}^{\mathrm{N}} \left(d_{\mathrm{d}}^2 + u_{\mathrm{s}}^2 + u_{\mathrm{t}}^2 \right) \qquad (2.30)$$

Where

d_d = directional term; 0 if in and 1 if out
u_s = ABS(V_F - V_S) / V_F (magnitude of velocity deviation)
u_t = (2/3k)$^{0.5}$ (turbulence intensity)
V_F = mean or nominal velocity at the face
V_S = face velocity for the ith cell on face
1/N is calculated by multiplying d_d, u_s and u_t by the cell volume and dividing by the box volume

The advantage of this calculation is that the performance is based on measurable parameters. The disadvantage is that the weighting of velocity, negative flow, and turbulence are equal, which is arbitrary.

2.5.3 Time to Reach Hood

As the flow into the hood is disrupted by the flow in the laboratory, the path of the air into the hood will be changed from that dominated by the suction of the hood. If the flow were a simple parallel flow into the sash opening, the mean time for air to reach each calculation point on the open face would be the distance (approximately 1 foot) divided by the air velocity, typically 100 fpm. The resulting mean time would be approximately 0.6 seconds. As the flow deviates due to room air motion the time into the hood will increase as a result of the longer path. The increase in time is a measure of the laboratory hood's performance in scavenging the working zone.

The advantage of this approach is that it is a simple measure of convective performance. It suffers from the lack of any measure of turbulent disruption.

2.5.4 Negative Flow

Three indices were defined in order to determine if the laboratory hood would be susceptible to leakage:

- The quantity and area of flow out through the plane, that is away from the laboratory hood creating leakage. If these are non-zero then the hood is leaking at that plane. The higher the value the higher the leakage rate.

- The quantity and area of negative flow if the airflow is temporarily disturbed by an air current 20% of the mean design face velocity. This index indicates the sensitivity of

the configuration to disturbances in the airflow around the hood either due to fluctuation in the ventilation system, or due to movement in the laboratory.

- The quantity and area of negative flow when the turbulence is acting in opposition to the inward flow. This index indicates the degree to which the level of turbulence is likely to overcome the inward convective flow.

These parameters are again simple and can be easily compared with measured data. However, as in the performance index, the combination of convective leakage (negative velocity) with turbulence is arbitrary.

2.5.5 Hood in Isolation

As a refinement of the Dalla Valle approach it was determined that the comparison of the flow should be made with the flow into an undisturbed laboratory hood, or hood in isolation, rather than that used in the Dalla Valle analysis, a perfect exhaust. The analysis program compares the flow in terms of:

- perpendicular velocity,
- air speed,
- turbulence intensity, and
- concentration.

At each plane of the working zone and the sash opening with that from a simulation of the hood in isolation. The higher the variation the greater the degree of disruption of the flow into the hood by the room configuration.

This approach could be considered an improvement on Dalla Valle in that it removes the hood design variation in flow by comparing it with the same hood in an otherwise undisturbed flow. The disadvantage of requiring a different reference for each hood design and sash opening still remains, making it difficult to compare different configurations.

2.5.6 Hood Leakage Factors

The analysis technique chosen for this research is based on a measure of the hood leakage. While the actual leakage experienced in practice will vary from one experiment to another due to variation in source size and rate. A factor can be derived

that indicates the relative leakage from a hood in a given configuration. Two primary factors have been defined:

The face leakage factor: The leakage from the hood face into the working zone. This is the mass flow rate of contaminant from inside the hood back against the flow through the sash opening and into the working zone, as a proportion of the total flow into the laboratory hood.

The box leakage ratio: The mass leakage from the working zone out into the laboratory divided by the mass leakage into the box through the sash. This represents the proportion of contamination from the hood that reaches the working zone that gets into the laboratory.

The mass leakage at any point comprises two constituent parts:

The outward convective flux is the sum for all negative velocities at the plane (e.g. the sash opening) of :

$$\sum \rho f_c V \qquad (2.31)$$

Where
ρ is the density of the contaminant
f_c is the fraction of concentration of the contaminant
V is the convective velocity perpendicular to the plane

The outward diffusive flux

$$D = \left(c_d / A\right) \times \left(f_2 - f_1\right) \qquad (2.32)$$

$c_d = A/[((\delta_1/2)/\Gamma_1) + ((\delta_2/2)/\Gamma_2)]$

Where
A is the area
f_1 and f_2 are the fractions of concentration inside and outside the plane.
δ_1 and δ_2 are the distances to the cell centers just inside and just outside the plane
Γ_1 and Γ_2 laminar plus turbulent viscosities / Schmidt No.

It is important to note that this cannot represent a pass-fail criterion since this does not account for either the source generation rate or the toxicity of the substance.

The advantage of this approach is that it directly addresses the potential for leakage from the hood. Thus different configurations can easily be compared. However, there is

a significant danger that the leakage predicted can be misinterpreted as an actual leakage, rather than a factor that represents the leakage from a completely contaminated hood. It is thus difficult to compare directly with empirical data.

A summary of the data calculated is presented for each configuration in the database of simulations in Volume II.

2.6 Nomenclature

ϕ' Fluctuating component of variable ϕ
$\bar{\phi}$ Mean component of variable ϕ
∂_{ij} Kronecker delta (1 if $i = j$ else = 0)
β Coefficient of thermal expansion
ρ Density
ε Rate of dissipation of turbulence energy
τ Shear stress
λ Thermal diffusivity
μ Viscosity
σ_T Turbulent Prandtl number
μ_{eff} Effective viscosity ($\mu + \mu_T$)
Γ_T Eddy diffusivity
μ_T Eddy viscosity
$C_{1\text{-}3,\mu}$ σ_k σ_ε Turbulence model constant(s)
g Acceleration due to gravity
H Enthalpy
k Turbulence energy
P Pressure
T Temperature
U_i Velocity tensor
x_i Distance tensor

2.7 CFD Glossary

Advection
The process by which a quantity of fluid is transferred from one point to another due to the movement of the fluid.

Boundary Condition(s)
either: A set of conditions that define the physical problem.

or: A plane at which a known solution is applied to the governing equations.

Boundary Layer
A very narrow region next to a solid object in a moving fluid, and containing high gradients in velocity.

CFD
Computational Fluid Dynamics. The study of the behavior of fluids using computers to solve the equations that govern fluid flow.

Clustering
Increasing the number of grid points in a region to better resolve a geometric or flow feature. Increasing the local grid resolution.

Continuum
Having properties that vary continuously with position. The air in a room can be thought of as a continuum because any cube of air will behave much like any other chosen cube of air.

Convection
A similar term to *Advection* but is a more generic description of the *Advection* process.

Convergence
Convergence is achieved when the imbalances in the governing equations fall below an acceptably low level during the solution process.

Diffusion
The process by which a quantity spreads from one point to another due to the existence of a gradient in that variable.

Diffusion, molecular
The spreading of a quantity due to molecular interactions within the fluid.

Diffusion, turbulent
The spreading of a quantity due to the increased mixing rates exhibited by turbulent flows. In the majority of situations turbulent diffusion far exceeds molecular diffusion.

Divergence
Divergence occurs when the imbalances in the governing equations reach unacceptably high levels during the solution process

Eddy viscosity

Eddy viscosity is an additional viscosity that is produced due to the effects of fluid turbulence.

Eddy diffusivity
Eddy diffusivity is the additional diffusivity produced due to the effects of fluid turbulence.

Far-field Distance
The approximate distance from the surface of the body to the farthest point in the Computational Domain. "The wing simulation had a far-field distance of 15 wing chords."

Gradient
The amount by which a variable changes in space or time.

Grid Resolution
The amount of grid points located in a physical area. "The grid uses 20 grid points to resolve the boundary layer".

Near-wall Spacing
The distance of the closest point to the surface of a body. An especially important parameter in viscous flow simulations.

Normal Stress
The force/unit area that results from one body directly striking another. For instance, slamming your fist down upon a table top will cause pain due to a normal stress on your hand and the table. Pressure is always a normal stress.

Reynolds number
A non-dimensional number that is used to indicate how turbulent a fluid flow is.

Reynolds stress
In turbulence modeling an instantaneous velocity is broken down into mean and fluctuating components. A Reynolds stress is the averaged product of two of these fluctuating velocity components.

Reynolds flux
A Reynolds flux, as in a Reynolds stress, is the average product of two fluctuating variable components, one of which is a fluctuating velocity component.

Shear Stress

The force/unit area that results from one body sliding relative to another. For instance, sliding a book along a table top will cause a shearing stress on both the book and table top.

Solution Domain
The computational volume in which the governing equations, together with the boundary conditions, are solved.

Turbulence
Turbulence is a type of flow that occurs when a fluid is moving quickly and / or within an unconfined space. It is characterized by a marked increase in mixing where, superimposed on the principle motion, there are countless irregular fluctuations.

Viscosity
The viscosity of a fluid is ascribed to the movement of one layer of fluid over another, i.e. a viscous fluid like maple syrup will take a long time to pour from a bottle, while beer can be poured quite readily. Viscosity is usually given the Greek symbol "μ". Water is about 100 times as viscous as air, while most oils are around 1000 times as viscous as water. The effects of viscosity are most easily related to a concept like friction. The viscosity of fluids will cause a resistance to motion, a drag, which must be overcome by providing more power. If the drag caused by viscosity is small compared to other forces, or if it is important only in a small region like in Boundary Layer Theory, then the effects of viscosity can be neglected. Such a case is called inviscid flow. It is a point of confusion, even for practicing aeronautical engineers, that an inviscid flow is not the flow of a fluid with zero viscosity, rather an inviscid flow contains negligibly small viscous stresses.

Vorticity
Vorticity is the swirling motion of a fluid. Satellite photographs on the evening news weather forecast often show large rotating masses of fluid, which are special cases of vortices.

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